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Engineering Cyclic Tetrapeptides Containing Chimeric Amino Acids as Preferred Reverse-Turn Scaffolds
Che, Y.; Marshall, G. R.

J. Med. Chem.; (Article); 2006; 49(1); 111-124. DOI: [10.1021/jm0507072](https://doi.org/10.1021/jm0507072)

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Neopetrosiamides, Peptides from the Marine Sponge *Neopetrosia* sp. That Inhibit Amoeboid Invasion by Human Tumor Cells

Williams, D. E.; Austin, P.; Diaz-Marrero, A. R.; Soest, R. V.; Matainaho, T.; Roskelley, C. D.; Roberge, M.; Andersen, R. J.

Org. Lett.; (Letter); 2005; 7(19); 4173-4176. DOI: [10.1021/ol051524c](https://doi.org/10.1021/ol051524c)

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Deazapurine Solid-Phase Synthesis: Construction of 3-Substituted Pyrrolo[3,2-*d*]pyrimidine-6-carboxylates on Cross-Linked Polystyrene Bearing a Cysteamine Linker

Rombouts, F. J. R.; Fridkin, G.; Lubell, W. D.

J. Comb. Chem.; (Article); 2005; 7(4); 589-598. DOI: [10.1021/cc050002l](https://doi.org/10.1021/cc050002l)

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Asymmetric Synthesis of 3-Substituted Proline Chimeras Bearing Polar Side Chains of Proteinogenic Amino Acids

Quancard, J.; Labonne, A.; Jacquot, Y.; Chassaing, G.; Lavielle, S.; Karoyan, P.

J. Org. Chem.; (Article); 2004; 69(23); 7940-7948. DOI: [10.1021/jo048762q](https://doi.org/10.1021/jo048762q)

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Virtually Complete Control of Simple and Face Diastereoselectivity in the Michael Addition Reactions between Achiral Equivalents of a Nucleophilic Glycine and (S)- or (R)-3-(*E*-Enoyl)-4-phenyl-1,3-oxazolidin-2-ones: Practical Method for Preparation of β -Substituted Pyroglutamic Acids and Prolines

Soloshonok, V. A.; Ueki, H.; Tiwari, R.; Cai, C.; Hruby, V. J.

J. Org. Chem.; (Article); 2004; 69(15); 4984-4990. DOI: [10.1021/jo0495438](https://doi.org/10.1021/jo0495438)

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Determinants of Corticotropin Releasing Factor. Receptor Selectivity of Corticotropin Releasing Factor Related Peptides

Mazur, A. W.; Wang, F.; Tscheiner, M.; Donnelly, E.; Isfort, R. J.

J. Med. Chem.; **(Article)**; **2004**; 47(13); 3450-3454. DOI: [10.1021/jm049883l](https://doi.org/10.1021/jm049883l)

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Restriction of a Peptide Turn Conformation and Conformational Analysis of Guanidino Group Using Arginine-Proline Fused Amino Acids: Application to Mini Atrial Natriuretic Peptide on Binding to the Receptor

Sugase, K.; Horikawa, M.; Sugiyama, M.; Ishiguro, M.

J. Med. Chem.; **(Brief Article)**; **2004**; 47(2); 489-492. DOI: [10.1021/jm030232j](https://doi.org/10.1021/jm030232j)

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Monitoring the Early Steps of Unfolding of Dicalcium and Mono-Ce³⁺-Substituted Forms of P43M Calbindin D_{9k}[†]

Jimenez, B.; Poggi, L.; Piccioli, M.

Biochemistry; **(Article)**; **2003**; 42(44); 13066-13073. DOI: [10.1021/bi034638+](https://doi.org/10.1021/bi034638+)

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Amino-Zinc-Enolate Carbometallation Reactions: Application to Ring Closure of Terminally Substituted Olefin for the Asymmetric Synthesis of *cis*- and *trans*-3-Prolinoleucine

Karoyan, P.; Chassaing, G.; Quancard, J.; Vaissermann, J.

J. Org. Chem.; **(Article)**; **2003**; 68(6); 2256-2265. DOI: [10.1021/jo026535n](https://doi.org/10.1021/jo026535n)

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☐ Current

Complex-Induced Proximity Effects. Temperature-Dependent Regiochemical Diversity in Lithiation-Electrophilic Substitution Reactions of *N*-BOC-2-Azabicyclo[2.1.1]hexane. 2,4- and 3,5-Methanoproline

Krow, G. R.; Herzon, S. B.; Lin, G.; Qiu, F.; Sonnet, P. E.

Org. Lett.; **(Letter)**; **2002**; 4(18); 3151-3154. DOI: [10.1021/ol026509b](https://doi.org/10.1021/ol026509b)

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☐ Current

Comparative Assessment of the Ligand and Metal Ion Binding Properties of Integrins $\alpha_9\beta_1$ and $\alpha_4\beta_1$

Pepinsky, R. B.; Mumford, R. A.; Chen, L. L.; Leone, D.; Amo, S. E.; Riper, G. V.; Whitty, A.; Dolinski, B.; Lobb, R. R.; Dean, D. C.; Chang, L. L.; Raab, C. E.; Si, Q.; Hagmann, W. K.; Lingham, R. B.
Biochemistry; **(Article)**; **2002**; 41(22); 7125-7141. DOI: [10.1021/bi020024d](https://doi.org/10.1021/bi020024d)

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☐ Current

The Rearrangement Route to 3-CH₂X-2-azabicyclo[2.1.1]hexanes. Substituent Control of Neighboring Group Participation

Krow, G. R.; Yuan, J.; Lin, G.; Sonnet, P. E.

Org. Lett.; **(Letter)**; **2002**; 4(8); 1259-1262. DOI: [10.1021/ol020007g](https://doi.org/10.1021/ol020007g)

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High Selectivity from Configurational Match/Mismatch in Carbon-Hydrogen Insertion Reactions of Steroidal Diazoacetates Catalyzed by Chiral Dirhodium(II) Carboxamidates

Doyle, M. P.; Davies, S. B.; May, E. J.

J. Org. Chem.; **(Article)**; **2001**; 66(24); 8112-8119. DOI: [10.1021/jo015932f](https://doi.org/10.1021/jo015932f)

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☐ Current

Synthesis of Conformationally Constrained Arginine and Ornithine Analogues Based on the 3-Substituted Pyrrolidine Framework

Mammi, A.; Hughes, N. E.; Wurthmann, A.; Madaleno, J. S.

J. Org. Chem.; **(Note)**; **2001**; 66(19); 6483-6486. DOI: [10.1021/jo010242x](https://doi.org/10.1021/jo010242x)

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☐ Current

Carbon-Carbon Bond-Forming Solid-Phase Reactions. Part II

Sammelson, R. E.; Kurth, M. J.

Chem. Rev.; **(Review)**; **2001**; 101(1); 137-202. DOI: [10.1021/cr000086e](https://doi.org/10.1021/cr000086e)

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☐ Current

Rational Design of Highly Diastereoselective, Organic Base-Catalyzed, Room-Temperature Michael Addition Reactions¹

Soloshonok, V. A.; Cai, C.; Hruby, V. J.; Meervelt, L. V.; Yamazaki, T.

J. Org. Chem.; **(Article)**; **2000**; 65(20); 6688-6696. DOI: [10.1021/jo0008791](https://doi.org/10.1021/jo0008791)

Abstract Full: [HTML](#) / [PDF](#) (121k) [Supporting Information](#)

☐ Current

Comprehensive Survey of Combinatorial Library Synthesis: 1999

Dolle, R. E.

J. Comb. Chem.; **(Review)**; **2000**; 2(5); 383-433. DOI: [10.1021/cc000055x](https://doi.org/10.1021/cc000055x)Full: [HTML](#) / [PDF](#) (1905k)☐ Current**Peptide and Peptide Mimetic Inhibitors of Antigen Presentation by HLA-DR Class II MHC Molecules.****Design, Structure-Activity Relationships, and X-ray Crystal Structures**

Bolin, D. R.; Swain, A. L.; Sarabu, R.; Berthel, S. J.; Gillespie, P.; Huby, N. J. S.; Makofske, R.; Orzechowski, L.; Perrotta, A.; Toth, K.; Cooper, J. P.; Jiang, N.; Falcioni, F.; Campbell, R.; Cox, D.; Gaizband, D.; Belunis, C. J.; Vidovic, D.; Ito, K.; Crowther, R.; Kammlott, U.; Zhang, X.; Palermo, R.; Weber, D.; Guenot, J.; Nagy, Z.; Olson, G. L.

J. Med. Chem.; **(Article)**; **2000**; 43(11); 2135-2148. DOI: [10.1021/jm000034h](https://doi.org/10.1021/jm000034h)Abstract Full: [HTML](#) / [PDF](#) (524k) [Supporting Information](#)☐ Current**Conformationally Constrained Substance P Analogues: The Total Synthesis of a Constrained Peptidomimetic for the Phe⁷-Phe⁸ Region**

Tong, Y.; Fobian, Y. M.; Wu, M.; Boyd, N. D.; Moeller, K. D.

J. Org. Chem.; **(Article)**; **2000**; 65(8); 2484-2493. DOI: [10.1021/jo991649t](https://doi.org/10.1021/jo991649t)Abstract Full: [HTML](#) / [PDF](#) (273k) [Supporting Information](#)☐ Current**Total Synthesis of Gypsetin, Deoxybrevianamide E, Brevianamide E, and Tryprostatin B: Novel Constructions of 2,3-Disubstituted Indoles**

Schkeryantz, J. M.; Woo, J. C. G.; Siliphaivanh, P.; Depew, K. M.; Danishefsky, S. J.

J. Am. Chem. Soc.; **(Article)**; **1999**; 121(51); 11964-11975. DOI: [10.1021/ja9925249](https://doi.org/10.1021/ja9925249)Abstract Full: [HTML](#) / [PDF](#) (401k) [Supporting Information](#)☐ Current**Stereoselective Reactions of *N*-(9-Phenylfluoren-9-yl)-4-oxoproline Enolates. An Expedient Route for the Preparation of Conformationally Restricted Amino Acid Analogues**

Blanco, M.-J.; Paleo, M. R.; Penide, C.; Sardina, F. J.

J. Org. Chem.; **(Article)**; **1999**; 64(24); 8786-8793. DOI: [10.1021/jo990283h](https://doi.org/10.1021/jo990283h)Abstract Full: [HTML](#) / [PDF](#) (112k)☐ Current**Synthesis and Serotonergic Activity of 3-[2-(Pyrrolidin-1-yl)ethyl]indoles: Potent Agonists for the h5-HT_{1D} Receptor with High Selectivity over the h5-HT_{1B} Receptor**

Sternfeld, F.; Guiblin, A. R.; Jelley, R. A.; Matassa, V. G.; Reeve, A. J.; Hunt, P. A.; Beer, M. S.; Heald, A.; Stanton, J. A.; Sohal, B.; Watt, A. P.; Street, L. J.

J. Med. Chem.; **(Article)**; **1999**; 42(4); 677-690. DOI: [10.1021/jm9805687](https://doi.org/10.1021/jm9805687)

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Design of Peptidomimetics That Inhibit the Association of Phosphatidylinositol 3-Kinase with Platelet-Derived Growth Factor- β Receptor and Possess Cellular Activity

Eaton, S. R.; Cody, W. L.; Doherty, A. M.; Holland, D. R.; Panek, R. L.; Lu, G. H.; Dahring, T. K.; Rose, D. R.
J. Med. Chem.; **(Article)**; **1998**; 41(22); 4329-4342. DOI: [10.1021/jm9802766](#)

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Stereoselective Synthesis of Tilivalline¹

Nagasaka, T.; Koseki, Y.

J. Org. Chem.; **(Article)**; **1998**; 63(20); 6797-6801. DOI: [10.1021/jo972158g](#)

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2-Nitrophenylcarbamoyl-(S)-prolyl-(S)-3-(2-naphthyl)alanyl-N-benzyl-N-methylamide (SDZ NKT 343), a Potent Human NK₁ Tachykinin Receptor Antagonist with Good Oral Analgesic Activity in Chronic Pain

Models

Walpole, C.; Ko, S. Y.; Brown, M.; Beattie, D.; Campbell, E.; Dickenson, F.; Ewan, S.; Hughes, G. A.; Lemaire, M.; Lerpiniere, J.; Patel, S.; Urban, L.

J. Med. Chem.; **(Article)**; **1998**; 41(17); 3159-3173. DOI: [10.1021/jm970499g](#)

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Tandem Asymmetric Cyclopropanation/Cope Rearrangement. A Highly Diastereoselective and Enantioselective Method for the Construction of 1,4-Cycloheptadienes

Davies, H. M. L.; Stafford, D. G.; Doan, B. D.; Houser, J. H.

J. Am. Chem. Soc.; **(Article)**; **1998**; 120(14); 3326-3331. DOI: [10.1021/ja974201n](#)

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A Novel Stereodivergent Synthesis of Optically Pure *cis*- and *trans*-3-Substituted Proline Derivatives

Sasaki, N. A.; Dockner, M.; Chiaroni, A.; Riche, C.; Potier, P.

J. Org. Chem.; **(Addition/Correction)**; **1997**; 62(26); 9388-9388. DOI: [10.1021/jo9740249](#)

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☐ Current

Potent $\alpha_4\beta_1$ Peptide Antagonists as Potential Anti-Inflammatory Agents

Jackson, D. Y.; Quan, C.; Artis, D. R.; Rawson, T.; Blackburn, B.; Struble, M.; Fitzgerald, G.; Chan, K.; Mullins, S.; Burnier, J. P.; Fairbrother, W. J.; Clark, K.; Berisini, M.; Chui, H.; Renz, M.; Jones, S.; Fong, S.
J. Med. Chem.; **(Article)**; **1997**; 40(21); 3359-3368. DOI: [10.1021/jm970175s](https://doi.org/10.1021/jm970175s)

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The Calyxolanes: New 1,3-Diphenylbutanoid Metabolites Isolated from the Caribbean Marine Sponge *Calyx podatypa*^{1,2}

Rodriguez, A. D.; Cobar, O. M.; Padilla, O. L.

J. Nat. Prod.; **(Note)**; **1997**; 60(9); 915-917. DOI: [10.1021/np970215v](https://doi.org/10.1021/np970215v)

Abstract Full: [HTML](#) / [PDF](#) (155k)

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Enantiodivergent Chemoenzymatic Synthesis of (*R*)- and (*S*)- β -Proline in High Optical Purity

Mazzini, C.; Lebreton, J.; Alphand, V.; Furstoss, R.

J. Org. Chem.; **(Note)**; **1997**; 62(15); 5215-5218. DOI: [10.1021/jo9701905](https://doi.org/10.1021/jo9701905)

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☐ Current

A Novel Stereodivergent Synthesis of Optically Pure *cis*- and *trans*-3-Substituted Proline Derivatives

Sasaki, N. A.; Dockner, M.; Chiaroni, A.; Riche, C.; Potier, P.

J. Org. Chem.; **(Note)**; **1997**; 62(3); 765-770. DOI: [10.1021/jo961790r](https://doi.org/10.1021/jo961790r)

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Naturally Occurring Proline Analogues

Mauger, A. B.

J. Nat. Prod.; **(Review)**; **1996**; 59(12); 1205-1211. DOI: [10.1021/np9603479](https://doi.org/10.1021/np9603479)

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Total Synthesis of Tryprostatin B: Generation of a Nucleophilic Prenylating Species from a Prenylstannane

Depew, K. M.; Danishefsky, S. J.; Rosen, N.; Sepp-Lorenzino, L.

J. Am. Chem. Soc.; **(Communication)**; **1996**; 118(49); 12463-12464. DOI: [10.1021/ja962954o](https://doi.org/10.1021/ja962954o)

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Asymmetric Nitroalkene [4 + 2] Cycloadditions: Enantioselective Synthesis of 3-Substituted and 3,4-

Disubstituted Pyrrolidines

Scott E. Denmark, Lawrence R. Marcin

J. Org. Chem.; **1995**; 60(10); 3221-3235.First Page Full: [PDF](#) (3422k)

☐ Current**Development of a Model for the .delta. Opioid Receptor Pharmacophore. 1. Conformationally Restricted Tyr1 Replacements in the Cyclic .delta. Receptor Selective Tetrapeptide Tyr-c[D-Cys-Phe-D-Pen]OH (JOM-13)**

Henry I. Mosberg, Andrei L. Lomize, Chenguang Wang, Heather Kroona, Deborah L. Heyl, Katarzyna Sobczyk-Kojiro, Wenli Ma, Carol Mousigian, Frank Porreca

J. Med. Chem.; **1994**; 37(25); 4371-4383.First Page Full: [PDF](#) (1824k)

☐ Current**Bicyclic Hydantoins with a Bridgehead Nitrogen. Comparison of Anticonvulsant Activities with Binding to the Neuronal Voltage-Dependent Sodium Channel**

Wayne J. Brouillette, Vladimir P. Jestkov, Milton L. Brown, M. Shamim Akhtar, Timothy M. DeLorey, George B. Brown

J. Med. Chem.; **1994**; 37(20); 3289-3293.First Page Full: [PDF](#) (579k)

☐ Current**Design and Synthesis of Side-Chain Conformationally Restricted Phenylalanines and Their Use for Structure-Activity Studies on Tachykinin NK-1 Receptor**

Hubert Josien, Solange Lavielle, Alie Brunissen, Monique Saffroy, Yvette Torrens, Jean-Claude Beaujouan, Jacques Glowinski, Gerard Chassaing

J. Med. Chem.; **1994**; 37(11); 1586-1601.First Page Full: [PDF](#) (2369k)

☐ Current**A conformational study by proton NMR of a cyclic pentapeptide antagonist of endothelin**

Murray Coles, Victoria Sowemimo, Denis Scanlon, Sharon L. A. Munro, David J. Craik

J. Med. Chem.; **1993**; 36(18); 2658-2665.First Page Full: [PDF](#) (1033k)

☐ Current**A [3+2] cycloaddition and [4+3] cycloaddition approach to N-heterocycles via palladium-catalyzed TMM reactions with imines**

Barry M. Trost, Christopher M. Marrs

J. Am. Chem. Soc.; **1993**; 115(15); 6636-6645.First Page Full: [PDF](#) (1234k)

☐ Current**Synthesis and biological activity of CCK heptapeptide analogs. Effects of conformational constraints and**

standard modifications on receptor subtype selectivity, functional activity in vitro, and appetite suppression in vivo

Mark W. Holladay, Michael J. Bennett, Michael D. Tufano, C. W. Lin, Karen E. Asin, David G. Witte, Thomas R. Miller, Bruce R. Bianchi, A. L. Nikkel, et al.

J. Med. Chem.; **1992**; 35(16); 2919-2928.

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☐ Current**Synthesis of .alpha.-benzyl .gamma.-lactam, .alpha.-benzyl .delta.-lactam, and .alpha.-benzylproline derivatives as conformationally restricted analogs of phenylalaninamide**

Mark W. Holladay, Alex M. Nadzan

J. Org. Chem.; **1991**; 56(12); 3900-3905.

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☐ Current**trans-3-n-propyl-L-proline is a highly favorable, conformationally restricted replacement for methionine in the C-terminal tetrapeptide of cholecystokinin. Stereoselective synthesis of 3-allyl- and 3-n-propyl-L-proline derivatives from 4-hydroxy-L-proline**

Mark W. Holladay, Chun Wei Lin, Catherine S. May, David S. Garvey, David G. Witte, Thomas R. Miller, Caroline A. W. Wolfram, Alex M. Nadzan

J. Med. Chem.; **1991**; 34(1); 455-457.

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☐ Current**Electrophilic olefin heterocyclization in organic synthesis. Highly stereoselective synthesis of trans 3,5-disubstituted pyrrolidin-2-ones by iodolactamization via homoallylic asymmetric induction**

Hiroki Takahata, Tamotsu Takamatsu, Yinshan Chen, Naoki Ohkubo, Takao Yamazaki, Takefumi Momose, Tadamasa Date

J. Org. Chem.; **1990**; 55(12); 3792-3797.

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☐ Current**Conformationally constrained amino acids. Synthesis and optical resolution of 3-substituted proline derivatives**

John Y. L. Chung, James T. Wasicak, William A. Arnold, Catherine S. May, Alex M. Nadzan, Mark W. Holladay

J. Org. Chem.; **1990**; 55(1); 270-275.

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☐ Current**Synthesis of 4-substituted prolines as conformationally constrained amino acid analogs**

Ari M. P. Koskinen, Henry Rapoport

J. Org. Chem.; **1989**; 54(8); 1859-1866.

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Formation of furylpyrrolidines and -piperidines on heating L-proline with reducing sugars and furancarboxaldehydes

Bernd Helak, Evelyn Kersten, Kurt Spengler, Roland Tressl, Dieter Rewicki
J. Agric. Food Chem.; **1989**; 37(2); 405-410.

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☐ Current

Formation of 7H-cyclopenta[b]pyridin-7-ones as proline-specific Maillard products

Bernd Helak, Kurt Spengler, Roland Tressl, Dieter Rewicki
J. Agric. Food Chem.; **1989**; 37(2); 400-404.

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☐ Current

Potent, long-acting luteinizing hormone releasing hormone antagonists containing new synthetic amino acids: N,N'-dialkyl-D-homoarginines

John J. Nestor, Jr., Ram Tahiramani, Teresa L. Ho, Georgia I. McRae, Brian H. Vickery
J. Med. Chem.; **1988**; 31(1); 65-72.

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☐ Current

Friedel-Crafts acylation with N-(trifluoroacetyl)-.alpha.-amino acid chlorides. Application to the preparation of .beta.-arylalkylamines and 3-substituted 1,2,3,4-tetrahydroisoquinolines

J. Eric Nordlander, Mark J. Payne, F. George Njoroge, Michael A. Balk, George D. Laikos, Vasanth M. Vishwanath
J. Org. Chem.; **1984**; 49(22); 4107-4111.

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☐ Current

Synthesis of dihydromauritine A, a reduced cyclopeptide alkaloid

Ruth F. Nutt, Kau Ming Chen, Madeleine M. Joullie
J. Org. Chem.; **1984**; 49(6); 1013-1021.

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☐ Current

Antihypertensive agents: angiotensin converting enzyme inhibitors. 1-[3-(Acylothio)-3-arylpropionyl]-L-prolines

Francis J. McEvoy, Fong M. Lai, J. Donald Albright
J. Med. Chem.; **1983**; 26(3); 381-393.

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☐ Current

Pyridazinones. 2. Synthesis and antisecretory and antiulcer activities of thiourea and 2-cyanoguanidine derivatives

Toshihiro Yamada, Youichi Nobuhara, Hiroshi Shimamura, Yoshitsugu Tsukamoto, Kazuo Yoshihara, Azuma Yamaguchi, Masahiko Ohki

J. Med. Chem.; **1983**; 26(3); 373-381.

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☐ Current

Synthesis and stereochemistry of 3-hydroxy-5-methylproline, a new naturally occurring imino acid

Anthony B. Mauger, Oswald A. Stuart, Edward Katz, Kaarin T. Mason

J. Org. Chem.; **1977**; 42(6); 1000-1005.

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agreement. Please note that this agreement limits use to scientific
research. Use for software development or design or implementation
of commercial gateways or other similar uses is prohibited and may
result in loss of user privileges and other penalties.

* * * * * STN Columbus * * * * *

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 11:19:07 ON 05 JAN 2006

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 4 JAN 2006 HIGHEST RN 871209-00-6

DICTIONARY FILE UPDATES: 4 JAN 2006 HIGHEST RN 871209-00-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

```
*****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005. A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*
*****
```

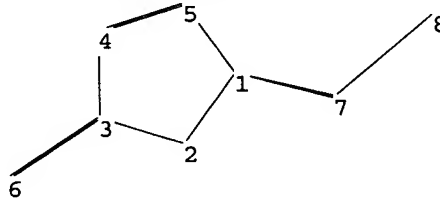
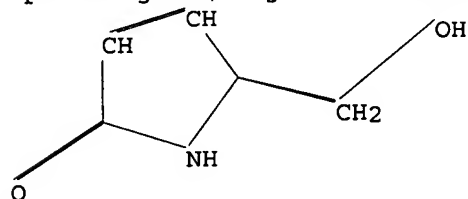
Structure search iteration limits have been increased. See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10821793\Struc 2.str



chain nodes :

6 7 8

ring nodes :

1 2 3 4 5

chain bonds :

1-7 3-6 7-8

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

Page 40

1-2 1-5 2-3 3-4 3-6 4-5
exact bonds :
1-7 7-8

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS

Stereo Bonds:

7-1 (Single Wedge).

Stereo Chiral Centers:

1 (Parity=Don't Care)

Stereo RSS Sets:

Type=Relative (Default). 1 Nodes= 1

L1 STRUCTURE UPLOADED

=> l1

SAMPLE SEARCH INITIATED 11:19:20 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2128 TO ITERATE

94.0% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 39793 TO 45327
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> l1 full

FULL SEARCH INITIATED 11:19:28 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 43131 TO ITERATE

100.0% PROCESSED 43131 ITERATIONS
SEARCH TIME: 00.00.01

1 ANSWERS

L3 1 SEA SSS FUL L1

=> d hitstr

'HITSTR' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN
SAM - Index Name, MF, and structure - no RN
FIDE - All substance data, except sequence data
IDE - FIDE, but only 50 names
SQIDE - IDE, plus sequence data
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
SQD - Protein sequence data, includes RN

SQD3 - Same as SQD, but 3-letter amino acid codes are used
SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties
EPROP - Table of experimental properties
PROP - EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract
APPS -- Application and Priority Information
BIB -- CA Accession Number, plus Bibliographic Data
CAN -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND -- Index Data
IPC -- International Patent Classification
PATS -- PI, SO
STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented

OBIB ----- AN, plus Bibliographic Data (original)
OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations
SIBIB ----- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.

The MAX format is the same as ALL.

The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):rn sam
'SAM' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN
SAM - Index Name, MF, and structure - no RN
FIDE - All substance data, except sequence data
IDE - FIDE, but only 50 names
SQIDE - IDE, plus sequence data
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
SQD - Protein sequence data, includes RN
SQD3 - Same as SQD, but 3-letter amino acid codes are used
SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties
EPROP - Table of experimental properties

PROP - EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract
APPS -- Application and Priority Information
BIB -- CA Accession Number, plus Bibliographic Data
CAN -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND -- Index Data
IPC -- International Patent Classification
PATS -- PI, SO
STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented

OBIB ----- AN, plus Bibliographic Data (original)
OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations
SIBIB ----- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.

The MAX format is the same as ALL.

The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):d rn sam
'SAM' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
'D' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN
SAM - Index Name, MF, and structure - no RN
FIDE - All substance data, except sequence data
IDE - FIDE, but only 50 names
SQIDE - IDE, plus sequence data
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
SQD - Protein sequence data, includes RN
SQD3 - Same as SQD, but 3-letter amino acid codes are used
SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties
EPROP - Table of experimental properties
PROP - EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats

must be cited first. The CA File predefined formats are:

ABS -- Abstract
 APPS -- Application and Priority Information
 BIB -- CA Accession Number, plus Bibliographic Data
 CAN -- CA Accession Number
 CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
 IND -- Index Data
 IPC -- International Patent Classification
 PATS -- PI, SO
 STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels
 IBIB -- BIB, indented, with text labels
 ISTD -- STD format, indented

OBIB ----- AN, plus Bibliographic Data (original)
 OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations
 SIBIB ----- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.

The MAX format is the same as ALL.

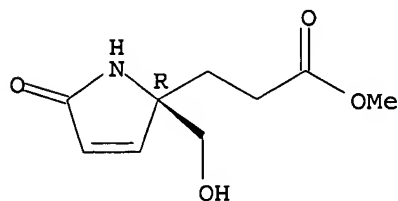
The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.
 HELP FORMATS -- To see detailed descriptions of the predefined formats.
 ENTER DISPLAY FORMAT (IDE):sam

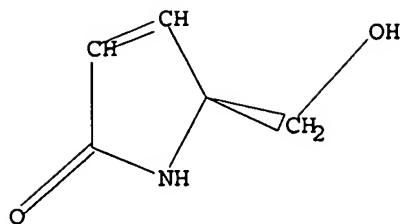
L3 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
 IN 1H-Pyrrole-2-propanoic acid, 2,5-dihydro-2-(hydroxymethyl)-5-oxo-, methyl ester, (R)- (9CI)
 MF C9 H13 N O4

Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

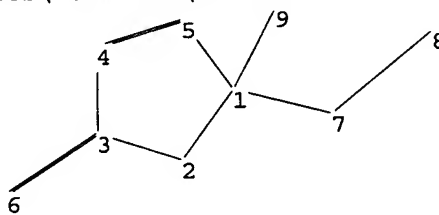
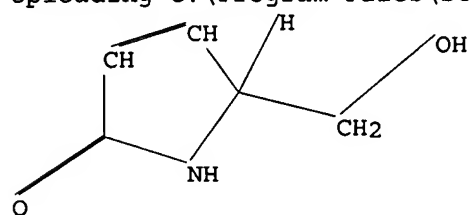
=> d 11
 L1 HAS NO ANSWERS
 L1 STR



Structure attributes must be viewed using STN Express query preparation.

=>

Uploading C:\Program Files\Stnexp\Queries\10821793\Struc 3.str



chain nodes :

6 7 8 9

ring nodes :

1 2 3 4 5

chain bonds :

1-7 1-9 3-6 7-8

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 2-3 3-4 3-6 4-5

exact bonds :

1-7 1-9 7-8

Match level :

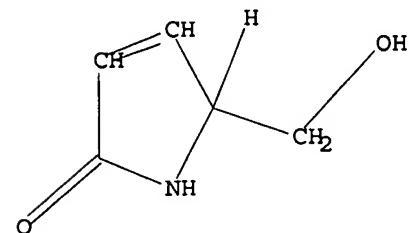
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS

L4 STRUCTURE UPLOADED

=> d 14

L4 HAS NO ANSWERS

L4 STR



Structure attributes must be viewed using STN Express query preparation.

=> l4

SAMPLE SEARCH INITIATED 11:22:00 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2128 TO ITERATE

94.0% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 39793 TO 45327
PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4

=> l4 full

FULL SEARCH INITIATED 11:22:07 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 43131 TO ITERATE

100.0% PROCESSED 43131 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L6 0 SEA SSS FUL L4

=> log y

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	336.58	336.79

STN INTERNATIONAL LOGOFF AT 11:22:44 ON 05 JAN 2006